Cryptohermitian Hamiltonians on graphs.

II. Hermitizations.

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Abstract

Non-hermitian quantum graphs possessing real (i.e., in principle, observable) spectra are studied via their discretization. The discretized Hamiltonians are assigned, constructively, an elementary pseudometric and/or a more complicated metric. Both these constructions make the Hamiltonian Hermitian, respectively, in an auxiliary (Krein or Pontryagin) vector space or in a less friendly (but more useful) Hilbert space of quantum mechanics.

1 Introduction

In paper I [1], Schrödinger equation $H\psi(x) = E\psi(x)$ with a non-Hermitian Hamiltonian $H = -\triangle + V \neq H^\dagger$ living on a non-tree toy-model graph $\mathbb{G}$ has been considered. We emphasized there that the unusual support $\mathbb{G}$ of H may find its multiple motivations in physics using slightly smeared or non-local interactions.

In mathematical context we paid attention to the meaning of the concept of the solvability of similar models. We proposed that the latter concept finds its most natural interpretation in the availability of the spectrum of energies in a sufficiently transparent form. For this purpose we replaced the "input" phenomenological Hamiltonian H by an infinite family of its discrete approximants $H^{(N)}$ and showed that and how this may simplify the underlying secular equation via its factorization. In this manner we were able to address the key problem emerging in similar quantum graph models, namely, the problem of the specification of the domain $\mathcal{D}$ of coupling constants for which the whole spectrum remains real.

In our present continuation of paper I we intend to show that for the couplings lying inside domain $\mathcal{D}$, all of the apparently non-Hermitian Hamiltonians $H^{(N)}$ with $N \leq \infty$ may be reinterpreted as Hermitian. In the first, preparatory step (cf. section 2) we shall recall some basic references and summarize a few relevant details of quantum theory. We shall also restrict our attention to the sufficiently elementary toy models with a feasible specification of the domain $\mathcal{D}$ of the reality (i.e., observability) of the energies.

In section 3 we shall describe the construction of a pseudo-metric $\mathcal{P}$ which obeys the relation

$$H^\dagger \mathcal{P} - \mathcal{P} H = 0 \tag{1}$$

and which will make our Hamiltonian pseudo-Hermitian, i.e., $\mathcal{P}-$self-adjoint in a suitable *ad hoc* Krein or, more precisely, Pontryagin space.

In section 4 a Dyson's map Ω will be assumed to exist inside $\mathcal{D}$, leading

to an isospectral avatar $\mathfrak{h} = \Omega\, H\, \Omega^{-1}$ of our Hamiltonian (cf., e.g., review [2] for more details). By construction, the latter operator proves self-adjoint in a certain "paternal" Hilbert space $\mathcal{H}^{(P)}$. In this context we shall remind the readers that the latter representation space is, in practice, never used for performing calculations. Its role is purely auxiliary. Its existence just enables us to translate the Hermiticity of $\mathfrak{h}$ in $\mathcal{H}^{(P)}$ into the equivalent concept of the "hidden Hermiticity" of our original Hamiltonian in a unitarily equivalent representation space $\mathcal{H}^{(S)}$ which is Hamiltonian-dependent and which is constructed here *ad hoc*.

In the context of quantum physics the latter type of construction has been first employed by Scholts, Geyer and Hahne [3]. It has multiple merits. In Hilbert space $\mathcal{H}^{(S)}$, for example, one can write relation $H = H^\ddagger$ (= hidden Hermiticity or "cryptohermiticity" of H) where the new conjugate $H^\ddagger$ is defined as an operator similar to $H^\dagger$. This similarity is mediated by the metric operator defined as the product $\Theta = \Omega^\dagger\Omega$ of Dyson's map with its conjugate. In our final section 5 we emphasize these connections and add a few further relevant comments and commentaries.

2 Discrete quantum graphs

In the abstract formalism of Quantum Mechanics the argument $x \in \mathcal{Q}$ of wave function $\psi(x)$ may play the role of an entirely formal variable. It need not necessarily be connected to a point-particle position or momentum. Besides its more exotic but still very traditional role of the time in quantum clocks [4] (where the set $\mathcal{Q}$ still coincides with the real line) it may even be chosen complex. For example, in the whole family of the so called $\mathcal{PT}-$symmetric quantum models the most convenient set $\mathcal{Q}$ is being chosen in the form of a left-right symmetric complex curve $\mathcal{C}(s)$ (cf. several recent reviews [5] of this innovative subject). In the so called quantum toboggans this curve may even run over several Riemann sheets of the wave function [6].

By its philosophy, paper I was closely related to the latter new theoretical developments. It offered a compact review of certain potentially useful new family of quantum models where the set $\mathcal{Q}$ is to be specified in the form of a suitable topologically nontrivial (though still just real) graph $\mathbb{G}$. In the present continuation of the short and sketchy text of paper I we are going to complement the message. In particular, we intend to explain how the exotic-looking quantum-graph models of paper I fit in the standard textbook formalism of quantum mechanics.

In a compact summary of the contents of paper I we have to recall that its mathematics was based on an $N-$point discretization $\mathcal{Q}^{(N)}$ of the original graph-shaped "kinematical" set $\mathcal{Q}$. The promising physical implications of the less usual choice of dynamics (i.e., of the interactions) has been motivated there by a resulting short-ranged observational nonlocality of the models in question. On constructive level the main attention of paper I (as well as of our older paper [7]) was devoted to the influence of topological nontriviality of graphs $\mathcal{Q}^{(N)}$ (or, ultimately [8], of their continuous-graph limits $\mathcal{Q}^{(\infty)}$) upon the factorizations of the secular equations as well as upon the reality and structure of the resulting spectra.

In the direction outlined in the conclusions of paper I we shall now turn attention to the next task of the analysis. This task has two aspects. On a purely formal level it lies just in a very straightforward replacement of the "false" Hilbert space $\mathcal{H}^{(F)}$ by the "standard" Hilbert space $\mathcal{H}^{(S)}$ (we use the notation proposed in [2]). This transition converts the *manifestly non-Hermitian* Hamiltonian operator $H \neq H^\dagger$ acting in $\mathcal{H}^{(F)}$ into its *manifestly Hermitian* version acting in $\mathcal{H}^{(S)}$.

On a less formalistic level one has to emphasize that the initial Hamiltonians H are only considered at the so called physical parameters, i.e., for the domains of couplings $\mathcal{D}^{(N)}$ which comply with the requirement that all the energies remain real and also, for the sake of simplicity of the discussion,

non-degenerate. In this sense the main task of the users of operators H lies in the specification of the standard Hilbert-space representation $\mathcal{H}^{(S)}$, i.e., in the *explicit construction* of the above-mentioned metric operator $\Theta = \Theta(H)$.

In the context of quantum theory on graphs, just the most elementary samples of H and Θ were shown obtainable in the tree-graph elementary models of paper [9]. In what follows we intend to complement this construction by the less trivial samples of the quantum graphs which combine the topological, mathematical nontriviality of the corresponding supportive sets $\mathcal{Q}^{(N)}$ with the expected phenomenological nontriviality of the resulting spectra of energies.

2.1 Runge-Kutta-type discretizations

In many papers dealing with concrete applications of Quantum Theory the feasibility of practical model-building is based on a suitable discretization of the spatial continuum (cf., e.g., Ref. [8] in this setting). In particular, in our papers [10, 11, 12] we considered one-dimensional Schrödinger equations and replaced (i.e., approximated) the underlying intervals of coordinates [say, $x \in (-\infty, \infty)$ or $x \in (-L, L)$] by suitable Runge-Kutta-type equidistant lattices of points x_k numbered by an integer subscript $k = \ldots, -1, 0, 1, \ldots$.

One of the most natural dynamical simulations of a *global*, long-ranged nonlocality is given by the replacement of the standard straight-line *real* interval of $x \in (-L, L)$ in one dimension (with either $L < \infty$ or $L = \infty$) by a tree-shaped graph. The resulting planar, spatial or hyperspatial metric graph can be assigned a toy-model Hamiltonian matrix.

A fairly large class of Hamiltonians admits not only a constructive pseudo-Hermitization (i.e., a fully non-numerical reconstruction of pseudometrics $\mathcal{P} = \mathcal{P}(H)$) but also a constructive pseudo-Hermitization (i.e., a fully non-numerical reconstruction of positive definite metrics $\Theta = \Theta(H)$), in a large subdomain of the domain of parameters where the spectrum is real. In

the absence of any interaction and for the finite number of the Runge-Kutta lattice points such an idea leads merely to the discrete version of the standard and solvable square-well model [11]. It may be perceived, say, as living on the linear discrete lattice of $N = 2K+1$ points,

$$\boxed{\boxed{\xi_{-K}}}\ \xi_{-K+1}\ \ldots\ \xi_{-2}\ \xi_{-1}\ \boxed{\boxed{\xi_0}}\ \xi_1\ \xi_2\ \ldots\ \xi_{K-1}\ \boxed{\boxed{\xi_K}}\ . \tag{2}$$

In terminology of Ref. [9] the three marked points ξ_{-K}, ξ_0 and ξ_K may be reinterpreted as three vertices of a discretized two-pointed-star graph $\mathbb{G}^{(2)}$. In the same spirit one can reinterpret the corresponding quantum square well as a discrete quantum graph [13] in which the dynamics of the system is controlled by $(2K+1)-$dimensional matrix Schrödinger equation

$$\left[\begin{array}{ccccccc}
2 & -1 & 0 & \ldots & & \ldots & 0\\
-1 & 2 & -1 & 0 & \ldots & \ldots & 0\\
0 & -1 & 2 & -1 & \ddots & & \vdots\\
\vdots & \ddots & \ddots & \ddots & \ddots & 0 & 0\\
 & & & -1 & 2 & -1 & 0\\
\vdots & & & \ddots & -1 & 2 & -1\\
0 & \ldots & & \ldots & 0 & -1 & 2
\end{array}\right]
\left[\begin{array}{c}
\psi(\xi_{-K})\\
\psi(\xi_{-K+1})\\
\psi(\xi_{-K+2})\\
\vdots\\
\psi(\xi_{K-1})\\
\psi(\xi_K)
\end{array}\right]
= E
\left[\begin{array}{c}
\psi(\xi_{-K})\\
\psi(\xi_{-K+1})\\
\psi(\xi_{-K+2})\\
\vdots\\
\psi(\xi_{K-1})\\
\psi(\xi_K)
\end{array}\right] . \tag{3}$$

In a generalization of such a model one can replace the trivial linear graph

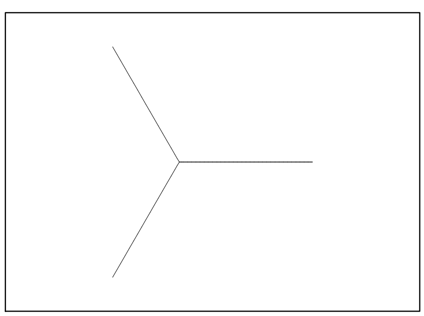

Figure 1: Star-shaped graph $\mathbb{G}^{(q)}$ with $q = 3$.

$\mathbb{G}^{(2)}$ by the three-pointed-star graph $\mathbb{G}^{(3)}$ of Fig. 1 with three wedges and four vertices. After a discretization such a graph coincides with the T-shaped

lattice

$$
\begin{array}{c}
\boxed{x_{N-2}}\ x_{N-5}\ \ldots\ x_5\ x_2\ \boxed{x_0}\ x_3\ x_6\ \ldots\ x_{N-4}\ \boxed{x_{N-1}}\\
x_1\\
x_4\\
\vdots\\
\boxed{x_{N-3}}
\end{array}
\qquad (4)
$$

In Ref. [9] we studied all the Schrödinger equations living on the $q-$pointed-star graphs at arbitrary q. In a move beyond the traditional model-building framework we followed the theory summarized in [2] and introduced a new concept of a non-Hermitian quantum graph. In our present paper we intend to move to some topologically less trivial quantum graphs.

2.2 Non-tree graphs

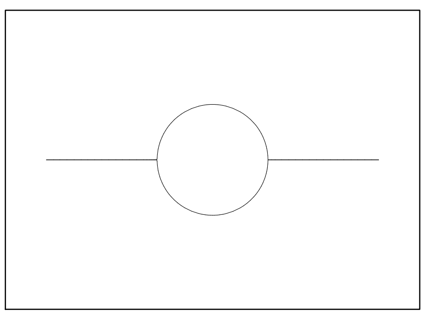

Figure 2: One of the simplest non-tree graphs.

In a purely numerical study [7] we replaced the topologically trivial graph of Fig. 1 by its scale-dependent loop-containing generalizations sampled by Fig. 2. We showed that similar quantum graphs still admit an efficient application of the Runge-Kutta-type discretization techniques.

The simplest family of discrete graphs contains the “loop” part is the

form which is next to trivial,

$$\begin{array}{ccccc} & \diagup & \boxed{x_{0^+}} & \diagdown & \\ \boxed{\boxed{x_{-K}}} - \ldots - \boxed{x_{-2}} - \boxed{\boxed{x_{-1}}} & & & & \boxed{\boxed{x_1}} - \boxed{x_2} - \ldots - \boxed{\boxed{x_K}} \,. \\ & \diagdown & \boxed{x_{0^-}} & \diagup & \end{array} \tag{5}$$

Just the number $2K$ of points of the symmetric pair of the external wedges can vary here. In the next step one can consider the lattices

$$\begin{array}{ccccc} & \diagup & \boxed{x_{U_1}} - \ldots - \boxed{x_{U_L}} & \diagdown & \\ \boxed{\boxed{x_{-K}}} - \ldots - \boxed{\boxed{x_{-1}}} & & & & \boxed{\boxed{x_1}} - \ldots - \boxed{\boxed{x_K}} \\ & \diagdown & \boxed{x_{D_1}} - \ldots - \boxed{x_{D_L}} & \diagup & \end{array} \tag{6}$$

containing the less trivial symmetric $2L-$point circular sublattice which represents the loop and opens the possibility of mimicking the the shape given by Fig. 2 in the limit of large $K, L \to \infty$.

2.3 Specific point-like interactions and their Hermiticity in disguise

In the spirit of Ref. [2] the physical meaning and standard probabilistic interpretation of *any* non-Hermitian Hamiltonian $H \neq H^\dagger$ with real spectrum may be derived from its Dyson-mapping-mediated Hermitian image $\mathfrak{h} = \Omega\, H\, \Omega^{-1}$. As a rule, operator $\mathfrak{h}$ is complicated by its form or counterintuitive by its origin. Otherwise, there would be no reason for turning attention to its isospectral-partner representation H. In this sense it is not surprising that in the quantum-graph models of Refs. [9, 10] the Dyson's operators Ω appeared to be fairly complicated.

Fortunately, the full knowledge of the latter operators is not too often

necessary in applications. The above-mentioned Hermiticity condition

$$\mathfrak{h} = \Omega\, H\, \Omega^{-1} = \mathfrak{h}^\dagger\,. \tag{7}$$

can be rewritten in the equivalent form of the Dieudonné's [14] hidden-Hermiticity constraint

$$H^\dagger = \Theta\, H\, \Theta^{-1}\,, \qquad \Theta = \Omega^\dagger \Omega\,. \tag{8}$$

We quite often need not factorize $\Theta \to \Omega$. After all, just the spectrum is usually sought and measured in experiments.

3 The Hermitization of Hamiltonians in Krein space

3.1 The choice of manifestly non-Hermitian interactions

In a way complementing the recent illustrative constructions [7, 15] let us turn attention to the non-tree graph of Fig. 2 and to one of its most elementary discrete versions or approximants

$$\boxed{x_{-2}} - \boxed{x_{-1}} \begin{array}{c} \diagup\, \boxed{x_{0+}} \,\diagdown \\ \\ \diagdown\, \boxed{x_{0-}} \,\diagup \end{array} \boxed{x_1} - \boxed{x_2}\,. \tag{9}$$

Once we endow its two central vertices x_{-1} and x_1 with a suitable non-Hermitian interaction we obtain the Hamiltonian

$$H(g,h;z) = \left[\begin{array}{cccccc} 2 & -1-z & & & & \\ -1+z & 3 & -1-g & -1-h & & \\ & -1+g & 2 & & -1+h & \\ & -1+h & & 2 & -1+g & \\ & & -1-h & -1-g & 3 & -1+z \\ & & & & -1-z & 2 \end{array} \right]$$

in which the unperturbed free-motion matrix $H(0,0;0)$ is not too different from its non-graph predecessor of Eq. (3). It is complemented by an elementary perturbation or interaction term which manifestly violates the Hermiticity.

In the language of physics the assignment of the three-parametric six-dimensional Hamiltonian $H(g,h;z)$ to the discrete graph (9) is directly inspired by Ref. [10] where we proposed that non-Hermitian interactions could simulate the presence of an elementary length in the theory. We emphasized in [10] that the current trends [16] of the introduction of the fundamental length are different, relating this quantity directly to certain hypothetical small anomalies in the geometry of the space or space-time. The internal bubble in our graph (9) can very naturally be reinterpreted as one of such anomalies. This returns us back to the mainstream literature where fundamental length proved relevant, e.g. in field theory [17], in string theory [18], in cosmology [19] or in astrophysics [20].

In our non-Hermitian models we can attribute the emergence of non-localities not only to the small bubbles in the real-line graph of coordinates but also to the smearing of space caused by the manifestly non-Hermitain interaction [9, 10, 15, 21]. A very similar idea appeared in preprint [22] where the concept of the nonvanishing fundamental length found its theoretical origin in a *combination* of the short-range spatial anomaly (viz.,

non-commutativity) *with* the smearing-effect of the Dyson-mapping Hermitization $H \to \mathfrak{h}$. One can expect model-building innovations of this type, say, in the context of the solid state phenomenology (cf. a sample of activities in this direction in Refs. [23]) or of the experimental optics [24] or, last but not least, of the recently revealed possibility of the formation of microscopic spatial subdomains with exotic properties in heavy-ion collisions [25].

3.2 Pseudometric $\mathcal{P}$ in a toy model - a non-numerical construction

One of the key sources of appeal of general non-Hermitian Hamiltonians $H \neq H^\dagger$ possessing real spectra may be traced back to letter [26] where Bender and Boettcher demonstrated the mind-boggling reality of the spectra for the whole one-parametric family of Hamiltonians $H = -\triangle + V^{(\varepsilon)}(x) \neq H^\dagger$ containing complex potentials $V^{(\varepsilon)}(x) = g^{(\varepsilon)}(x)x^2$ with $g^{(\varepsilon)}(x) = (\mathrm{i}x)^\varepsilon$. Tentatively they assigned their observations to the so called $\mathcal{PT}-$symmetry of their operators $H^{(\varepsilon)}$ and wave functions [5].

In the language of mathematics, $\mathcal{P}$ and $\mathcal{T}$ need not necessarily be just parity and time reversal operators as in [26]. Moreover, the $\mathcal{PT}-$symmetry of H should be rephrased as the property written in the form of Eq. (1) which may be called $\mathcal{P}-$ pseudo-Hermiticity and which has already been studied, many years ago, by mathematicians [14] as well as by physicists [27].

The most popular choice of $\mathcal{P}$ in the form of parity operator enables one to treat Eq. (1) as the $\mathcal{P}-$Hermiticity in a Krein space. We have shown in Refs. [9, 10] that for graph-supported Hamiltonians the search for a suitable operator $\mathcal{P}$ is much less trivial (though still feasible) and that one only has to speak about the $\mathcal{P}-$Hermiticity of H in a Pontryagin space. A *complete* set of the linearly independent sparse-matrix operators $\mathcal{P} = \mathcal{P}_n$ (compatible with Dieudonné's Eq. (1)) has successfully been assigned to a selected H in [10].

Table 1: Dozen nontrivial matrix elements of Eq. (1) after ansatz (10).

position	element to vanish	position	element to vanish
2	-b + b z + a + a z	7	-a - a z + b - b z
9	-e + e g - u + u h + b + b g	10	-u + u g - f + f h + b + b h
14	-b - b g + e - e g + u - u h	17	-c - c h + e - e h + u - u g
20	-b - b h + u - u g + f - f h	23	-c - c g + u - u h + f - f g
27	-e + e h - u + u g + c + c h	28	-u + u h - f + f g + c + c g
30	-d - d z + c - c z	35	-c + c z + d + d z

After we concentrate our attention to the discrete graph or lattice (5) with the growing number K of grid points on each external wedge, we have to imagine that besides the existing explicit (and mostly numerical) analyses of the spectra (sampled, say, in Refs. [1, 7]), one can be interested in the non-numerical aspects of these models. Thus, for our present quantum-graph sample Hamiltonian $H(g,h;z)$ let us search for its generalized parity via the most elementary nondiagonal ansatz

$$\mathcal{P} = \left[\begin{array}{cccccc} a & & & & & \\ & b & & & & \\ & & e & u & & \\ & & u & f & & \\ & & & & c & \\ & & & & & d \end{array} \right] . \qquad (10)$$

Its direct insertion in the Dieudonné's "hidden-Hermiticity" constraints (1) forms, in general, a set of 36 linear equations which have to be satisfied by the 21 unknown (and, say, real) matrix elements of the nondiagonal candidate $\mathcal{P}$ for the pseudometric. In such a situation the 24 linear relations (1) degenerate to identities and one is left just with the twelve nontrivial right-hand matrix-

element expressions summarized in Table 1.

Table 2: Eight matrix elements of Eq. (1) after the elimination of a and d.

position	element to vanish	position	element to vanish
9	-e + e g - u + u h + b + b g	10	-u + u g - f + f h + b + b h
14	-b - b g + e - e g + u - u h	17	-c - c h + e - e h + u - u g
20	-b - b h + u - u g + f - f h	23	-c - c g + u - u h + f - f g
27	-e + e h - u + u g + c + c h	28	-u + u h - f + f g + c + c g

All of these expressions have to be made equal to zero by the suitable choice of the unknown matrix elements in our ansatz for $\mathcal{P}$. As long as the 12 constraints of Table 1 are not all independent, we may employ the first one and the last one and eliminate

$$a = \frac{1-z}{1+z}\,b\,, \qquad d = \frac{1-z}{1+z}\,c\,.$$

The resulting reduced system of eight equations is summarized in Table 2.

The final matrix solution $\mathcal{P}$ of Eq. (1) can be normalized, say, by the choice of

$$u = 2\,.$$

This means that we arrive at the final four definitions of the unknowns,

$$e = f = g + h\,, \qquad b = \frac{2 + g - g^2 - h - h\,g}{1+g}\,, \qquad c = \frac{2 - g - h\,g + h - h^2}{1+h}\,.$$

One can immediately verify that the resulting matrix $\mathcal{P}$ is not positive definite. This means that it cannot be interpreted as a metric in Hilbert space but merely as an indefinite metric in an *ad hoc* specified and Hamiltonian-dependent Pontryagin space.

3.3 The lattice with any size $N = 2K + 2$

The symbolic-manipulation experience gained during the construction of $\mathcal{P}$ at $K = 2$ can be extended to all the higher integers $K \geq 3$ because we now know which matrix elements must be taken into account in relations (1). This facilitates the determination of the matrix elements of $\mathcal{P}$ at any $K \geq 3$ via an amended ansatz which leads to the final formulae.

Proposition 3.1. *For our quantum-graph Hamiltonians $H(g, h; z)$ of matrix dimension $N = 2K + 2$, there exists a non-diagonal solution $\mathcal{P}$ of Eq. (1) with the following non-vanishing matrix elements,*

$$\mathcal{P}_{K+1,K+2} = \mathcal{P}_{K+2,K+1} = 2\,, \qquad \mathcal{P}_{K+1,K+1} = \mathcal{P}_{K+2,K+2} = g + h\,,$$

$$\mathcal{P}_{2,2} = \mathcal{P}_{3,3} = \ldots = \mathcal{P}_{K,K} = \frac{2 + g - h - h\,g - g^2}{1 + g}\,,$$

$$\mathcal{P}_{2K+1,2K+1} = \mathcal{P}_{2K,2K} = \ldots = \mathcal{P}_{K+3,K+3} = \frac{2 + h - g - g\,h - h^2}{1 + h}$$

and

$$\mathcal{P}_{1,1} = \frac{1 - z}{1 + z}\mathcal{P}_{2,2}\,, \qquad \mathcal{P}_{2K+2,2K+2} = \frac{1 - z}{1 + z}\mathcal{P}_{2K+1,2K+1}\,.$$

Proof. The proof by insertion is straightforward. ☐

The conclusions extracted form the formulae obtained at $K = 2$ remain unchanged.

4 The Hermitization of Hamiltonians in Hilbert space

4.1 Positive-definite metric Θ in a toy model

The spectrum of our first nontrivial discrete quantum graph (9) with $K = 2$ is easily evaluated. It proves composed of the degenerate constant doublet $E_{\pm}^{(0)} = 2$ complemented by the quadruplet of certain coupling-dependent

energies. It is worth mentioning that once we reparametrize the couplings $g = \gamma + \delta$ and $h = \gamma - \delta$, we obtain the two series of energies

$$E_\pm^{(2)} = E_\pm^{(2)}(\gamma, z) = \frac{5}{2} \pm \frac{1}{2}\sqrt{21 - 16\,\gamma^2 - 4\,z^2}\,, \qquad (11)$$

$$E_\pm^{(1)} = E_\pm^{(1)}(\delta, z) = \frac{5}{2} \pm \frac{1}{2}\sqrt{5 - 16\,\delta^2 - 4\,z^2} \qquad (12)$$

where one of the parameters is always absent. This property is also exhibited by similar models at higher Ks [1].

The domain $\mathcal{D}$ of the admissible couplings (i.e., of the reality of the spectrum) will be rectangular at $z = 0$. For example, in the $K = 2$ domain $\mathcal{D}$ we shall have $\gamma \in (-\gamma_{(max)}, \gamma_{(max)})$ and $\delta \in (-\delta_{(max)}, \delta_{(max)})$, with $\gamma_{(max)} = \pm\sqrt{21/16}$ and $\delta_{(max)} = \pm\sqrt{5/16}$. Even when we choose $z \neq 0$ we can still use formulae (11) and (12) for a close-form specification of the so called "exceptional-point" boundary $\partial\mathcal{D}$ where the system ceases to be Hermitizable.

The three-parametric nature of domain $\mathcal{D}$ makes its description unnecessarily complicated, especially because the parameters g and h both describe just a certain asymmetry of the short-range interaction part of the Hamiltonian. For this reason let us now simplify the system and contemplate solely its $\delta = 0$ special cases with $H = H(g, g; z)$.

This restriction will certainly simplify the search for a metric matrix Θ which must necessarily be real and positive. The existence of such a matrix would immediately imply that some of the eligible Dyson's matrices Ω may also very easily be defined as the positive square roots of Θ.

An important advantage of reduction $g = h$ is that it results in the admissibility of $\Theta = \Theta^{(diagonal)}$. Even the naive symbolic-manipulation software

enables us to find $\Theta^{(diagonal)}$ in the rather clumsy form

$$\left[\begin{array}{cccccc} \frac{(1+g-(1+g)g)(1-z)}{(1+g)(1+z)} & & & & & \\ & \frac{1+g-(1+g)g}{1+g} & & & & \\ & & 1+g & & & \\ & & & 1+g & & \\ & & & & \frac{1+g-(1+g)g}{1+g} & \\ & & & & & \frac{(1+g-(1+g)g)(1-z)}{(1+g)(1+z)} \end{array} \right]. \tag{13}$$

This result can and has to be simplified "by hand".

Many non-diagonal matrices $\Theta = \Theta(H)$ may be constructed using symbolic-manipulation methods. In order to illustrate this possibility (which reflects just the well known ambiguity of the metric [3]) we can even proceed non-numerically, by combining our diagonal, parameter-free metric $\Theta^{(diag.)}$ of Eq. (13) with the pseudometric $\mathcal{P}$ of preceding section 3. This yields the one-parametric family of the nondiagonal candidates

$$\Theta(\alpha) = \Theta^{(diag.)} + \alpha\,\mathcal{P} \tag{14}$$

for the metric. The necessary restriction

$$\frac{1+g}{1-g} \;>\; 2\,\alpha \;>\; -1$$

guarantees that the resulting matrix $\Theta(\alpha)$ is positive definite and characterizes, therefore, the ultimate and sought one=parametric family of the alternative Hilbert spaces $\mathcal{H}^{(S)}(\alpha)$ of states with the non-equivalent but still entirely standard probabilistic physical interpretation. Naturally, these spaces differ by admitting *different* families of the other, complementary observables [3].

4.2 Matrix Hamiltonians of any size $N = 2K + 2$

Whenever one keeps all the free parameters inside domain $\mathcal{D}$ where, by definition, all the spectrum of energies is real, the corresponding $N-$dimensional

Hamiltonian matrix $H(g,h;z)$ may be considered isospectral to its Hermitian partner $\mathfrak{h}(g,h;z)$. According to the above-mentioned general recipe, the correct probabilistic interpretation of the Hamiltonian requires, therefore, that we find a solution $\Theta = \Theta(H)$ of the Dieudonné's hidden-Hermiticity condition, i.e., of the underdetermined linear set of equations (8).

In paragraph 4.1 we demonstrated that at $K = 2$ one must be a bit careful when using the computer-assisted symbolic manipulations. For this reason we employed an amended code and tested it on the $K = 3$ problem with the simplified $g = h$ Hamiltonian $H(g,g;z) =$

$$\left[\begin{array}{cccccccc}
2 & -1-z & & & & & & \\
-1+z & 2 & -1 & & & & & \\
 & -1 & 3 & -1-g & -1-g & & & \\
 & & -1+g & 2 & & -1+g & & \\
 & & -1+g & & 2 & -1+g & & \\
 & & & -1-g & -1-g & 3 & -1 & \\
 & & & & & -1 & 2 & -1+z \\
 & & & & & & -1-z & 2
\end{array}\right].$$

As the result we obtained the diagonal metric matrix with the following non-vanishing matrix elements,

$$\Theta^{(diagonal)}_{1,1} = \Theta^{(diagonal)}_{8,8} = \frac{(1-z)\,(1-g)}{1+z}\,,$$

$$\Theta^{(diagonal)}_{2,2} = \Theta^{(diagonal)}_{3,3} = \Theta^{(diagonal)}_{6,6} = \Theta^{(diagonal)}_{7,7} = 1-g\,,$$

$$\Theta^{(diagonal)}_{4,4} = \Theta^{(diagonal)}_{5,5} = 1+g\,,$$

specified up to an arbitrary overall constant factor. The knowledge of these formulae enables us to conclude that at least in the square-shaped domain with $|z| < 1$ and $|g| < 1$ all of the energies of the model remain real.

Although the similar recipe merely provides the sufficient condition of the reality of the energies, we see that it may cover large intervals of couplings. Similar quantum graphs with $g = h$ remain also tractable non-numerically

at the higher dimensions. Last but not least, at the larger values of K one better appreciates the difference between the dynamical roles of the "central" coupling g and the "asymptotic" coupling z [7]. Even the "first nontrivial" $K = 4$ Hamiltonian $H(g, g; z)$ represented by the ten-dimensional matrix

$$\left[\begin{array}{cccccccccc}
2 & -1-z & & & & & & & & \\
-1+z & 2 & -1 & & & & & & & \\
 & -1 & 2 & -1 & & & & & & \\
 & & -1 & 3 & -1-g & -1-g & & & & \\
 & & & -1+g & 2 & & -1+g & & & \\
 & & & -1+g & & 2 & -1+g & & & \\
 & & & & -1-g & -1-g & 3 & -1 & & \\
 & & & & & & -1 & 2 & -1 & \\
 & & & & & & & -1 & 2 & -1+z \\
 & & & & & & & & -1-z & 2
\end{array}\right]$$

illustrates this comment and enables us to reveal the general pattern. This opens the way towards non-numerical characteristics of Hamiltonians $H(g, g; z)$ at all the integers K and dimensions $N = 2K + 2$.

Proposition 4.1. *For the two-parametric subfamily of our quantum-graph Hamiltonians $H(g, g; z)$ of matrix dimension $N = 2K + 2L$ with $L = 1$ and with parameters g and z in a domain $\mathcal{D}^{(K,L)} \subset \mathcal{D}$, there exists a diagonal, positive solution $\Theta^{(K,L)}$ of Eq. (8) with the following non-vanishing matrix elements,*

$$\Theta^{(K,L)}_{2,2} = \Theta^{(K,L)}_{3,3} = \ldots = \Theta^{(K,L)}_{K,K} = 1 - g\,,$$

$$\Theta^{(K,L)}_{K+1,K+1} = \ldots = \Theta^{(K,L)}_{K+2L,K+2L} = 1 + g\,,$$

$$\Theta^{(K,L)}_{K+2L+1,K+2L+1} = \ldots = \Theta^{(K,L)}_{2K+2L-1,2K+2L-1} = 1 - g$$

and

$$\Theta^{(K,L)}_{1,1} = \Theta^{(K,L)}_{2K+2L,2K+2L} = \frac{(1-z)\,(1-g)}{1+z}\,.$$

Proof. The proof by insertions is straightforward. □

Remark 4.2. We did not encounter any essential obstacles when we tried to replace our Hamiltonians $H(g,g;z)$ living on the non-Hermitian discrete quantum graph (5) (where the inner loop contains just four points, viz., $x_{\pm 1}$ and $x_{0^\pm}$) by their generalizations living on similar discrete graphs containing $2L+2$ inner-loop points with $L = 2, 3, \ldots$. In this sense also the applicability and validity of Proposition 4.1 may be extended accordingly.

Remark 4.3. Once we succeeded in finding *a* metric, our Hamiltonian $H(g,g;z)$ may be declared Hermitian in the corresponding Hilbert space $\mathcal{H}^{(S)}$. This means that its *spectrum* must *necessarily be real* inside *all* the domain $\mathcal{D}^{(K)} \subset \mathcal{D}$ where the positive-definite metric exists. Thus, the explicit construction of *some* Θ appears to be a fairly efficient method of the rigorous proof of the reality of the spectrum inside a subdomain of $\mathcal{D}$.

5 Discussion

We showed that the family of manifestly non-Hermitian discrete quantum graphs admits not only its pseudo-Hermitization (i.e., the construction of a certain generalized parity – or pseudo-metric – operator $\mathcal{P}$) but also its Hermitization (i.e., an explicit construction of metric Θ in some of the eligible "physical" or "standard" Hilbert spaces $\mathcal{H}^{(S)}$).

Our present quantum-graph-building strategy can be perceived as an ambitious realization of the innovative concept of spatial nonlocality at short distances. In our present text a specific non-tree graph realization of such a quantum structure has been addressed as a certain first-step study aimed at a broader future project. In our concrete, model-based analyses the structure of the short-range anomalies has only been mimicked by a single small loop. We believe that the transition to some more complicated graphs will not lead to any technical complications in the future.

One of the traditional technical obstacles related to the study of non-Hermitian Hamiltonians can be seen in their rather difficult perturbative (in)tractability [21]. We circumvented this obstacle by the discretization techniques. We have demonstrated that this trick facilitated not only the analysis of spectra but also the reconstruction of the metrics and pseudo-metrics.

Our text has been based on the presentation of Quantum Theory as summarized in review [2]. In essence, every operator of an observable quantity is assumed represented, *simultaneously*, in several auxiliary Hilbert spaces $\mathcal{H}_j$. In contrast to the current practice where only the unitarily equivalent Hilbert spaces are considered (often, these Hilbert spaces are connected by Fourier-type transformations), the innovated formalism requires that the underlying one-to-one transformations Ω (often called Dyson's mappings [3]) are not unitary so that, in general, just one of the spaces (say, $\mathcal{H}_0 = \mathcal{H}^{(phys)}$) is usually declared "physical".

Historical origins of such an idea date back to pure mathematics [14]. In physics, its repeated re-births were emerging in perturbation theory [27, 28], in the theory of heavy nuclei [3], in field theory [29], in quantum cosmology [30] etc. In all of these contexts one treats the state-vector $\psi(x)$ and/or the generator of its time evolution (i.e., Hamiltonian H) as quantities which only admit the correct physical interpretation after a transition to the auxiliary space $\mathcal{H}^{(P)}$ *or rather* to its unitarily equivalent and, generically, more friendly form $\mathcal{H}^{(S)}$ where the inner product is defined via nontrivial metric Θ.

The real popularity of such a formalism has been evoked by letters [26, 31] where the mind-boggling ambiguity of the metric has most efficiently been suppressed via an *ad hoc* requirement of a charge times parity times time-reflection symmetry of the Hamiltonian. This approach (carrying the historic [27] nickname of $\mathcal{PT}-$symmetric quantum theory [5]) should be perceived as a *maximally nonlocal* formulation of the theory. In Ref. [21] the identifi-

cation of the $\mathcal{PT}-$symmetry postulates with the extreme nonlocality of the operator of coordinate is in fact based on reference to paper Ref. [32] where such an "infinite-range" characterization of the models in question has been discovered in a slightly different context.

For this reason the $\mathcal{PT}-$symmetry-based recipe appeared entirely unsuitable for extension from its current and natural bound-state applications, say, to the sufficiently compact and transparent description of the unitary scattering (cf. the more detailed explanations in Ref. [33]). In the literature one finds two ways out of this difficulty. In one of them we simply *turn attention to open systems*. The necessary (e.g., Feshbach's projection) techniques and their implementations have been recently sampled in a long review paper [34] or in a very short preprint on lattice models [35]).

In our papers [7, 10] the second possibility has been investigated and endorsed. Now, we may formulate its extension ot the problem of scattering on graphs as the open problem for imminent analysis. The core of this new developments may be again expected to lie in the replacement of the maximally nonlocal $\mathcal{PT}-$symmetric recipe by *another guiding principle*. Requiring, in essence, that the range of the smearing of coordinates caused by the action of Θ (let us denote this fundamental length by the usual symbol θ) should be finite.

In the first preliminary application of this idea to bound states on quantum graphs in Ref. [9] the size of θ has been left unspecified. In a proposal of continuation of these studies the quantity θ should be understood as playing the role of a *phenomenological* length which measures the range of the not-too-nonlocal smearing of the measurements of coordinates attributed to the non-Hermiticity of the tentative interaction living on the graph.

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